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13. ABSTRACT (Maximum 200 words)

Time-dependent, multidimensional computations were performed to study basic issues related to the structure of shocks, detonations, and modes of combustion affecting the feasibility or performance of the ram accelerator. A focus was on understanding of the structure and stability of oblique detonations generated by oblique shocks in supersonic fuel-air mixtures. The simulations show that steady, oblique detonations can be stabilized in supersonic flows and that they have very complex, multidimensional stuctures. Basic elements of such detonation structure include: (1) a nonreactive, oblique shock, (2) an induction zone, (3) a set of deflagration waves, and (4) a "reactive shock" in which the shock front is closely coupled with the energy release. This structure is stable and resilient to disturbances in the flow in a wide range of flow and mixture conditions. The conditions under which the overall detonation structure becomes unstable have also been identified. Preliminary studies which compared extremely resolved Navier-Stokes simulations to a boundary-layer model indicate some fundamental disagreements between the model and the simulations which require further investigations to resolve.

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NUMERICAL STUDIES FOR THE RAM ACCELERATOR

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Background

In the ram accelerator [1,2], a projectile that resembles the center-body of a ramjet travels through a premixed fuel-air mixture. When the projectile travels at supersonic speeds, oblique shocks formed in the flow may ignite the mixture and lead to oblique detonations or other types of shock-induced combustion. High pressures generated by the combustion process can accelerate the projectile to very high speeds. Several features of this type of system make its design more advantageous than conventional systems. Unlike the rocket, there is neither an engine nor fuel on the moving projectile, and most of the energy is used to accelerate the payload. Also, contrary to conventional guns, the energy release and related pressure rise take place near the projectile and are distributed along the entire barrel. However, in order to maximize performance, combustion must be generated and stabilized at appropriate locations in the system. Therefore, successful development of such systems depends on knowledge of the shock-induced combustion and the related reactive flow structures in the ram accelerator.

Among different types of shock-induced combustion, oblique detonations offer the most rapid and efficient form of energy conversion. In a supersonic fuel-air mixture, when the temperature behind an oblique shock is high enough, combustion occurs very close to the shock front to form a detonation wave in which the pressure rise due to combustion is closely coupled to that of the shock. This provides a very promising alternative combustion mechanism particularly applicable in high Mach-number regimes ($M \geq 5.0$) where more conventional combustion mechanisms encounter difficulties. Previous studies [3-5] of oblique detonation waves indicate that stable oblique detonations can be established under appropriate flow conditions. However, the conditions under which stable oblique standing detonation waves exist were not yet defined, and the structure of oblique detonations in the ram accelerator was not clearly understood.

There are a number of factors that can affect the stability of a standing detonation. These include the material composition, the shape of the projectile, the velocity of the projectile, turbulent boundary layers that form on the projectile, and the size and geometry of the barrel. When the material is too energetic, the detonation becomes unstable; when it is not energetic enough, a detonation does not form. The shape and speed of the projectile determine where a standing shock will form and these, too, determine the location and stability of oblique detonations. Turbulent boundary layers may also affect the location of the standing shocks and detonations.

In the last three years, the Laboratory for Computational Physics and Fluid Dynamics has undertaken a computational investigation of the basic structure and dynamics of oblique detonations under conditions appropriate for ram accelerators. These studies have shown that [6-9]:

1. Over a wide range of mixture compositions and Mach numbers, steady, oblique detonations can be established on the projectile. Such oblique detonations are quite stable and very resiliant to disturbances in the flow field and, therefore, provide a good combustion mechanism under these flow and mixture conditions.
2. The fundamental structure of oblique detonations described in this work has since been confirmed by recent experiments [10,11].
3. If the temperature is not high enough to generate a detonation, as might occur for low Mach number flows or less energetic mixture compositions, the combustion region is decoupled from the shock front.
4. Some preliminary results were obtained in which extremely resolved Navier-Stokes computations were compared to less resolved computations using a Baldwin-Lomax turbulent boundary-layer model. The two types of computations agree to the extent that the boundary layer has the effect of strengthening and steepening the shock. However, the very large quantitative disagreements in the amount of steepening needs to be resolved.

Detailed Summary of Current Research

In the work performed to date on this project, we have concentrated on addressing the fundamental question concerning oblique detonations in the ram accelerator: Can the concept of using a stable, oblique detonation actually be viable for ram accelerators? To answer this, a number of more specific questions have been addressed:

1. What are the conditions under which such standing oblique detonations exist? How do they depend on mixture composition, inflow velocity, and the geometry of the projectile?
2. What is the structure of such an oblique detonation?
3. How stable is the structure to perturbations? What is the dynamic response of the structure to a perturbation?
4. What are the effects of viscosity and boundary layers on the structure?

In order to answer these questions, we studied supersonic mixtures of fuel and air that are flowing through shocks generated by the flow past wedges. The wedges are similar to the nose cone of the projectile, and the wedge angle controls the shock strength. The basic configration, as well as the computational domain, are shown on Figure 1. We have addressed the problem computationally using a two-dimensional time-dependent model that solves the compressible Navier-Stokes equations coupled to a model for chemical reactions and the associated energy release. The code used in this study consists of separate convection and chemistry modules. Each module can be independently activated to evaluate the contribution and relative importance of different processes. These modules are coupled together by the time-step splitting technique [12].

The convection part of the conservation equations is solved using the Flux-Corrected Transport (FCT) algorithm [13]. This algorithm is conservative and monotonic (positivity-preserving). Monotonicity is achieved by introducing a diffusive flux and later correcting the calculated results with an antidiffusive flux modified by a flux limiter. FCT is capable of accurately simulating flows containing multiple shocks and is particularly suitable to study detonation structures. This algorithm has been used to investigate many phenomena in reactive and nonreactive flows, including the development and dynamics of detonation cells in two-dimensional channels [14,15].

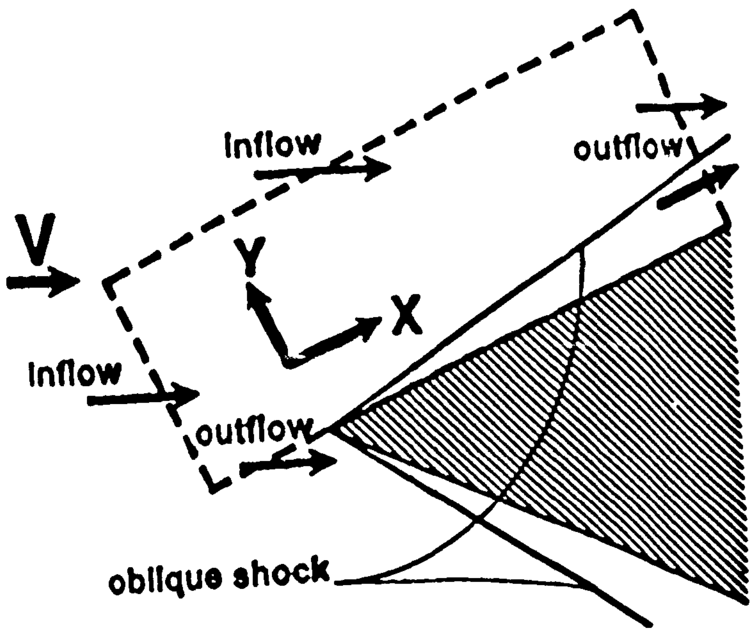


Figure 1. Schematic of the computational domain attached to a wedge surface.

A two-step reaction model is used to calculate the rates of the species production and energy release in the chemical reactions. In this model, the first step simulates the overall radical formation and accumulation, and the second step represents the formation of the final combustion products and associated energy release [15,16]. In the first step, a variable called the induction parameter is used to track the production and accumulation of the combustion radicals. This induction parameter is convected as a scalar variable. Then, its value in each computational cell is updated according to the production rate of the combustion radicals at the local temperature, pressure, and mixture ratio. These production rates were obtained from calculations using detailed reactions and tabulated for each flow and mixture condition. A fast table-look-up algorithm [15] is employed to allow these rates to be quickly accessed by the computational program. In the simulations, the induction parameter has normalized values from 0.0 (no combustion radicals) to 1.0 (beginning of the energy release).

We have focused the study on mixtures of hydrogen, oxygen, and nitrogen in mixture ratios ranging from 2:1:0 to 2:1:7. The Mach number of the inflow has ranged from Mach 5 to Mach 7. The pressure and temperature of the inflowing gas have been kept at 1 atm and 300 K. The wedge angle varies from 23 to 36 degrees.

In the computational domain shown in Figure 1, the inflow conditions are applied on the upper and left boundaries. The outflow conditions are imposed to the right and the first part of the lower boundary. The second part of the lower boundary, starting from a specified computational cell, is attached to the wedge surface. In this section, the slip condition is used for the inviscid calculations, and an adiabatic wall is assumed for viscous computations. The computational domain is extended far enough in the y-direction to insure that the inflow conditions used on the upper boundary do not interfere with flow structures generated on the wedge. However, figures presented in this paper show only the lower part of the computational domain, that is, the part containing the entire oblique shock and all shock-induced reactive structures. The number of computational cells ranges from 200×50 to 800×300, and the cell sizes are chosen according to the flow and mixture conditions.

Benchmark Nonreactive Shock-on-Wedge Studies

In order to validate the computational model, a series of nonreactive shocks generated on wedges were computed (Figure 2a). These studies showed that the shock angle and the flow properties behind the shock agree very well with the analytical solutions if the wedge angle is smaller than the critical flow-turning angle. Otherwise, the flow behind the shock is choked, and the shock continuously moves upstream (Figure 2b).

Basic Structure of Oblique Detonations

Figure 3 shows profiles of selected physical quantities from a simulation after the initial transient has passed and a steady, stable structure forms. The oblique shock has two different parts which have distinct shock angles. In the region near the leading edge of the wedge, the shock angle corresponds to the weak solution for a nonreactive shock through which the incoming flow turns 23° clockwise parallel to the wall. Behind this part of the shock, all fluid properties remain constant except the induction parameter. In this region, combustion radicals are being produced, and, therefore, the value of the induction parameter increases. The contours of water and temperature indicate that neither water formation nor energy release occurs in this induction region.

When the radical concentration in the flow becomes high enough to cause water formation and the associated energy release, the induction parameter becomes unity. This marks the end of the induction zone, and, behind this induction zone, water is produced, and the temperature and pressure begin to increase. As the heated mixture expands, the flow near the wall acquires a vertical velocity. This upward momentum pushes the flow away from the wall and effectively increases the wedge angle and, therefore, strengthens the upper part of the shock. This steepened shock produces substantially higher temperatures and sharply reduces the induction delay in the flow behind this part of the shock. When the induction delay becomes short enough, the oblique shock and the initiation of energy release are closely coupled. Behind the two different parts of the shock structure, the density, temperature, and velocity after the energy release are different due to the different shock strengths. The slip line that separates these two regions can be seen in the density and temperature contours.

For wide ranges of mixture and flow conditions, the simulations show a basic detonation structure generated by wedge-induced shocks. This essential configuration is independent of the flow and mixture conditions, although the scale of the structure may change by several orders of magnitude.

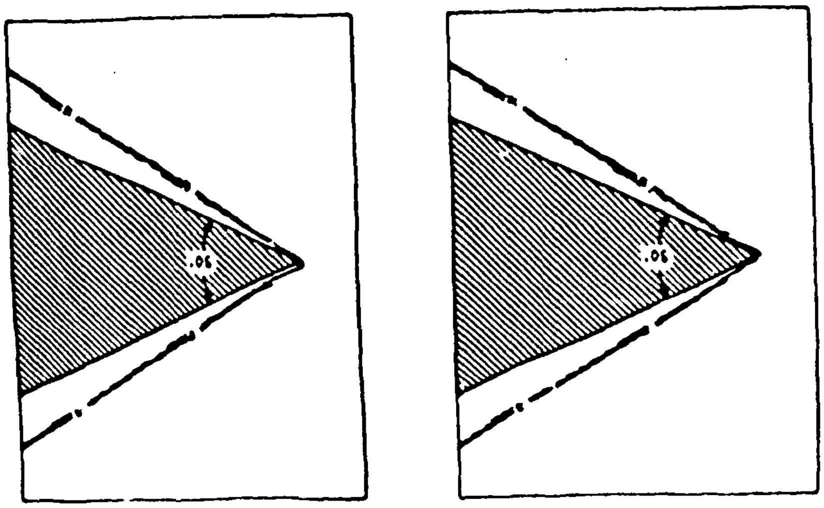
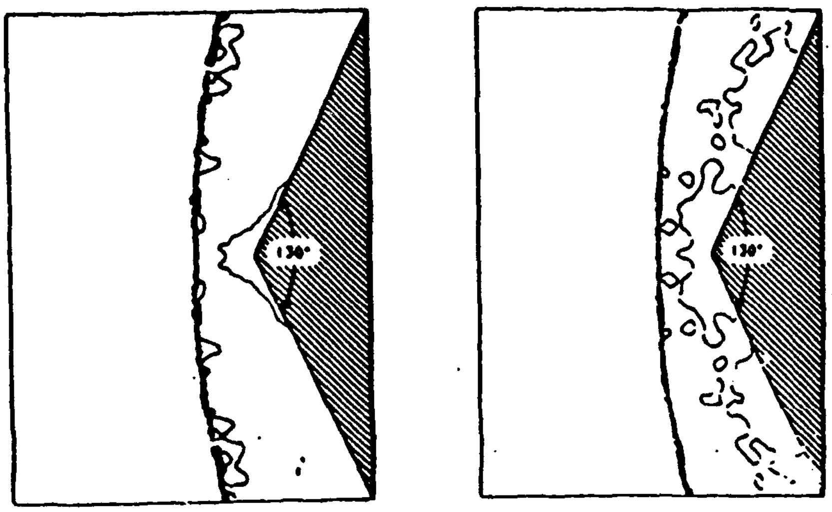


Figure 2a. Computed density contours for a supersonic flow passing by a wedge of 50 degrees from inviscid (left) and viscous (right) calculations. The inlet conditions are: density = 1.117 kg/m^3, pressure = 1.013 kPa, and Mach number = 8.

Figure 2b. Computed density contours for a supersonic flow passing by a wedge of 130 degrees from inviscod (left) and viscous (right) calculations. The inslet conditons are the same as those in Figure 2a.



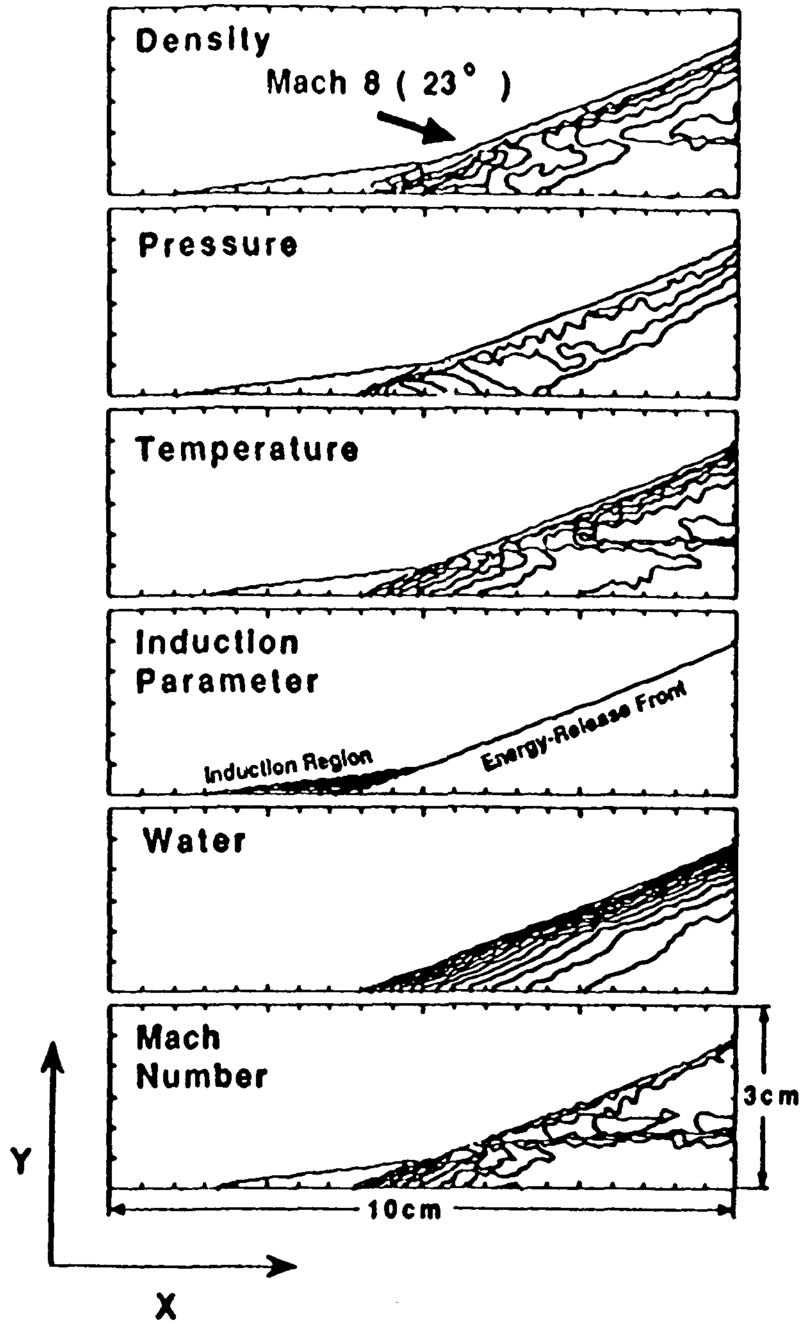


Figure 3. Contours from the simulation Mach 8 flow over a 23° wedge in the stoichiometric hydrogen-air mixture (H_2:O_2:N_2/2:1:3.76). The size of the computational domain is 10.0×3.75 cm^2 and the numerical resolution is $\Delta x = \Delta y = 0.025$ cm.

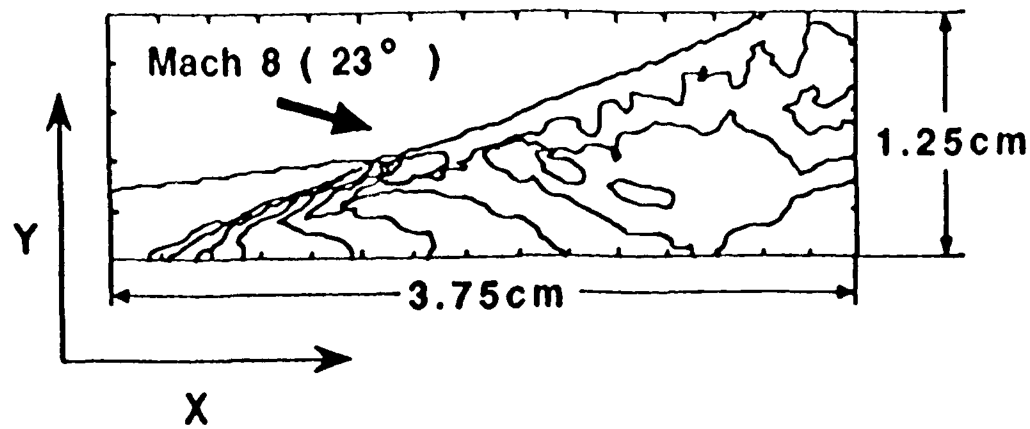


Figure 4. An enlarged pressure contour showing the detailed wave structures behind the induction zone from the simulation shown in Figure 3.

Figure 4a is an enlarged pressure contour that allows us to see the structure more clearly. There are a set of deflagration waves, generated by the energy release at the the end of the induction zone. Immediately above the wall, the energy release and the associated deflagration waves are separated from the shock front by a large distance which represents the induction delay. These deflagrations then propagate upward at the local Mach angle. The Mach angle becomes steeper for each successive deflagration wave due to the increasing temperature across these waves. Therefore, they gradually converge into each other. Also, the induction delay becomes shorter as these deflagration waves converge. Finally, the deflagrations intersect the shock front because the Mach angle of these deflagration waves is steeper than the nonreactive-shock angle in front of the induction region near the wall. Above the intersection, the energy release is coupled with the shock, and this upper, reactive shock is significantly steeper than the lower, nonreactive shock in front of the induction zone. This larger shock angle accommodates changes in the flow direction as well as the rapid heat release. The schematic in Figure 4b depicts the basic configuration of the detonation structure described above.

Resolution Requirements

The structure of the induction zone is crucial to the generation and stabilization of any reactive waves behind the shock. However, the length scale of the induction process is fairly short in the cases studied here and depends nonlinearly on the temperature, pressure, and composition of the mixture behind the shock. This scale decreases rapidly as temperature increases [16]. Unless the scale of the simulations or experimental measurements is small enough to resolve this distance, the detailed structure of the oblique detonations will not be correctly obtained.

In order to ensure that the computations are conducted with adequate resolution, four different grid resolutions, $\Delta x = \Delta y = 2.0$, 1.0, 0.5 and 0.25 mm, were tested for the case discussed above. Figure 5 shows enlargements of the induction region for all four resolutions. The two coarser resolutions (2.0 and 1.0 mm) show virtually instantaneous combustion within one or two computational cells. However, the two finer resolutions (0.5 and 0.25 mm) resolve the induction zone. In these simulations, inadequate resolution not only produces quantitatively inaccurate results, but also generates qualitatively incorrect physical features.

Detonation Structure in Different Mixtures

This basic structure of oblique detonations has been observed in a wide range of hydrogen-oxygen-nitrogen mixtures from 2:1:0 to 2:1:7 and for a range of wedge angles from 23 to 35 degrees. As the amount of nitrogen dilution decreases, the amount of energy released increases. This results in a higher temperature, greater speed of sound, and lower Mach number in the products of combustion. As a consequence, the reactive shock above the induction region becomes stronger, and the shock angle increases accordingly. When the amount of dilution is further decreased to zero, the shock angle is too large for the overall configuration to be stable, and the entire structure moves upstream continuously. A similar effect is observed when the wedge angle is increased while keeping the mixture proportions constant.

For the H_2:O_2:N_2 mixtures ranging from 2:1:7 to 2:1:1, the detonation structure is steady on the wedge. Figure 6 shows a simulation with no nitrogen (2:1:0) for which the detonation structure is no longer steady. The entire detonation structure moves continuously upstream and eventually impinges on the boundaries of the computational domain. In order to accommodate the upstream-moving, reactive shock, the computational domain is extended from 3.75 cm to 7.5 cm in the y-direction. In this case, increases in the shock strength and shock angle are more dramatic. Similar to the earlier cases, the density, temperature, and velocity of the mixtures are quite different in the two regions behind and above the induction zone due to the different shock strengths. Also, the velocity shear in this case is very strong, and there are some vortical structures generated by the Kelvin-Helmholtz instability along the slip line.

Effects of Shock Strength

When the shock strength is increased beyond a certain point (in this case, the wedge angle is increased), the oblique detonation also becomes unstable. Figure 7 shows a series of pressure and density contours for wedge angles ranging from 23° to 35° and for which the inflow temperature, density, and Mach number are not changed. The basic reactive structure described previously is observed in all cases shown here. Not only are the basic elements still intact, but the configurations of the detonation structures are geometrically similar. However, due to the variation in temperature and pressure behind the wedge-induced shock, the length of the induction region is very different in each case. For example, in the case of the 23° wedge, the temperature behind the shock is about 1200 K, and the induction distance is approximately 3 cm. In the cases of the 29° and 35° wedges, the temperatures are about 1400 K and 1700 K respectively, and the induction distances are reduced to the order of a millimeter and a tenth of a millimeter, respectively.

Stability of Oblique Detonations

The simulations described above demonstrate that an oblique detonation can be stabilized on a wedge. We then investigated the stability of such detonation structures and whether or not disturbances would significantly change the structures. The results of one such computation performed to answer this question are shown in Figure 8. In this simulation, a burning pocket is artifically introduced as a disturbance into the flow field originally computed for a stable detonation in a hydrogen-air mixture. This pocket is convected downstream and eventually merges with the original detonation structure, creating a larger and stronger detonation. However, the changes in the structure caused by the disturbance are eventually convected out of the computational domain,

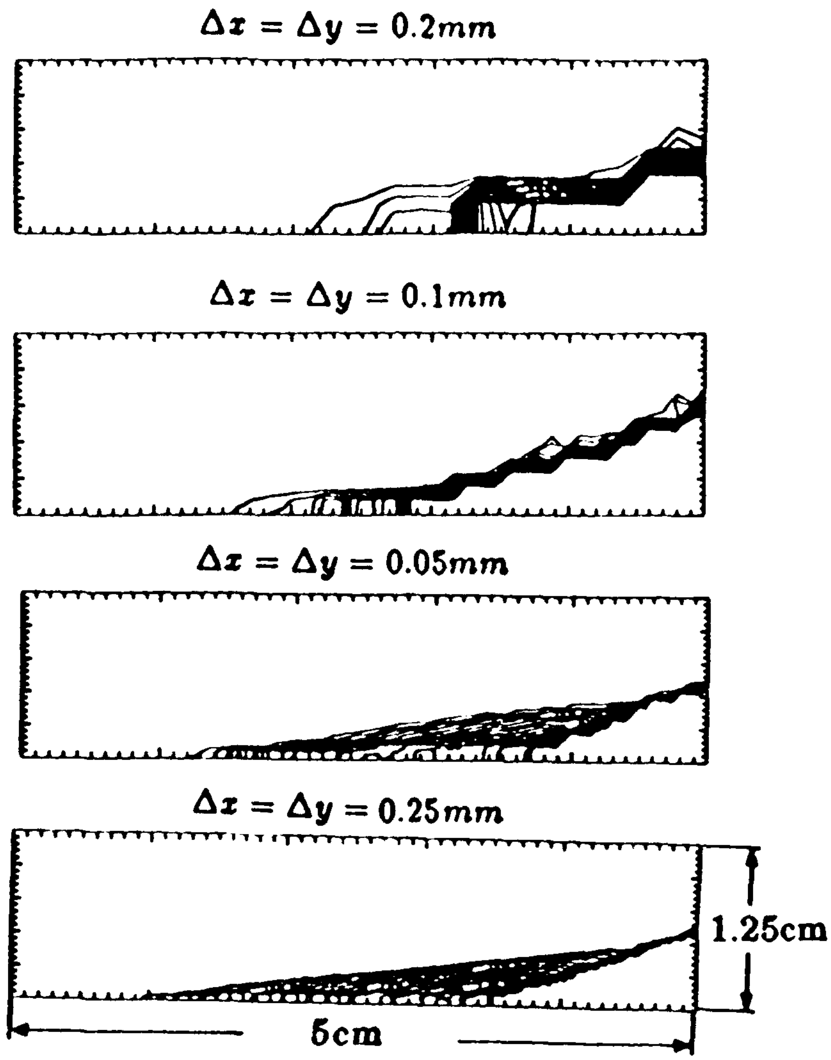


Figure 5. Computed induction zones from simulations using different grid resolutions.

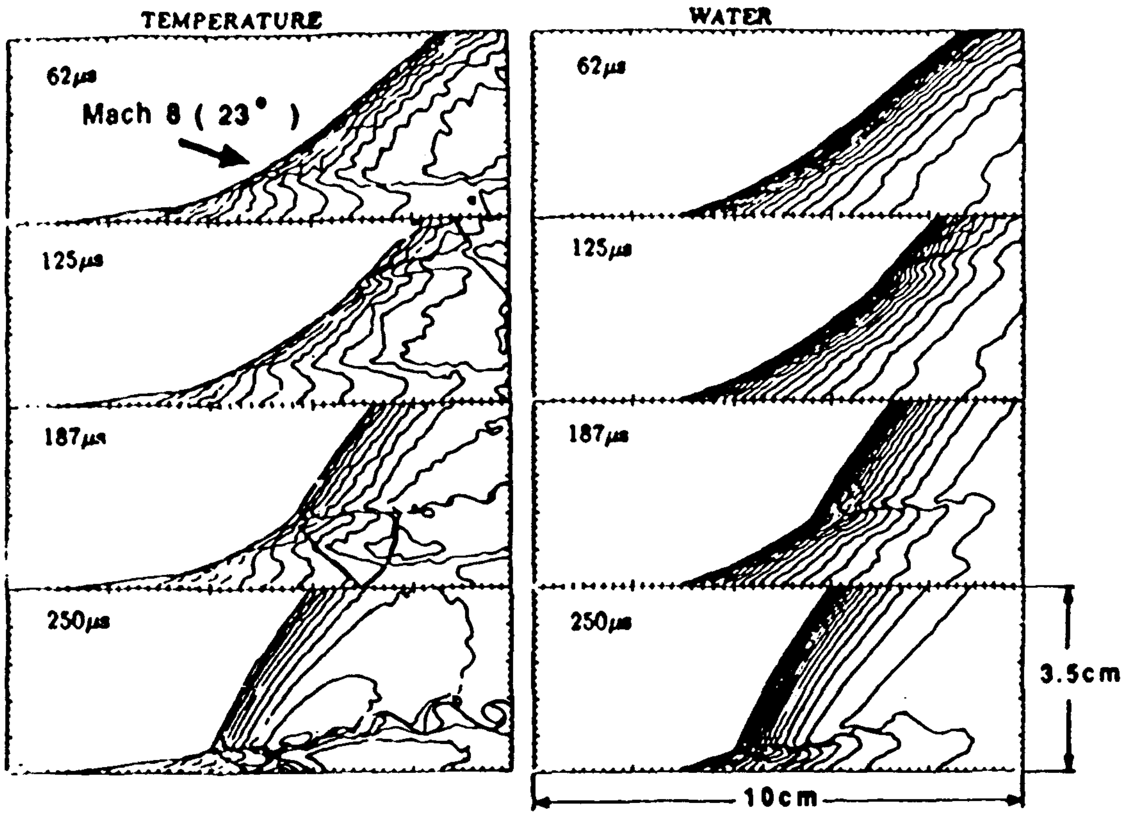


Figure 6. Development of an unsteady detonation structure on a 23° wedge in the stoichiometric hydrogen-oxygen mixture (H_2:O_2/2:1).

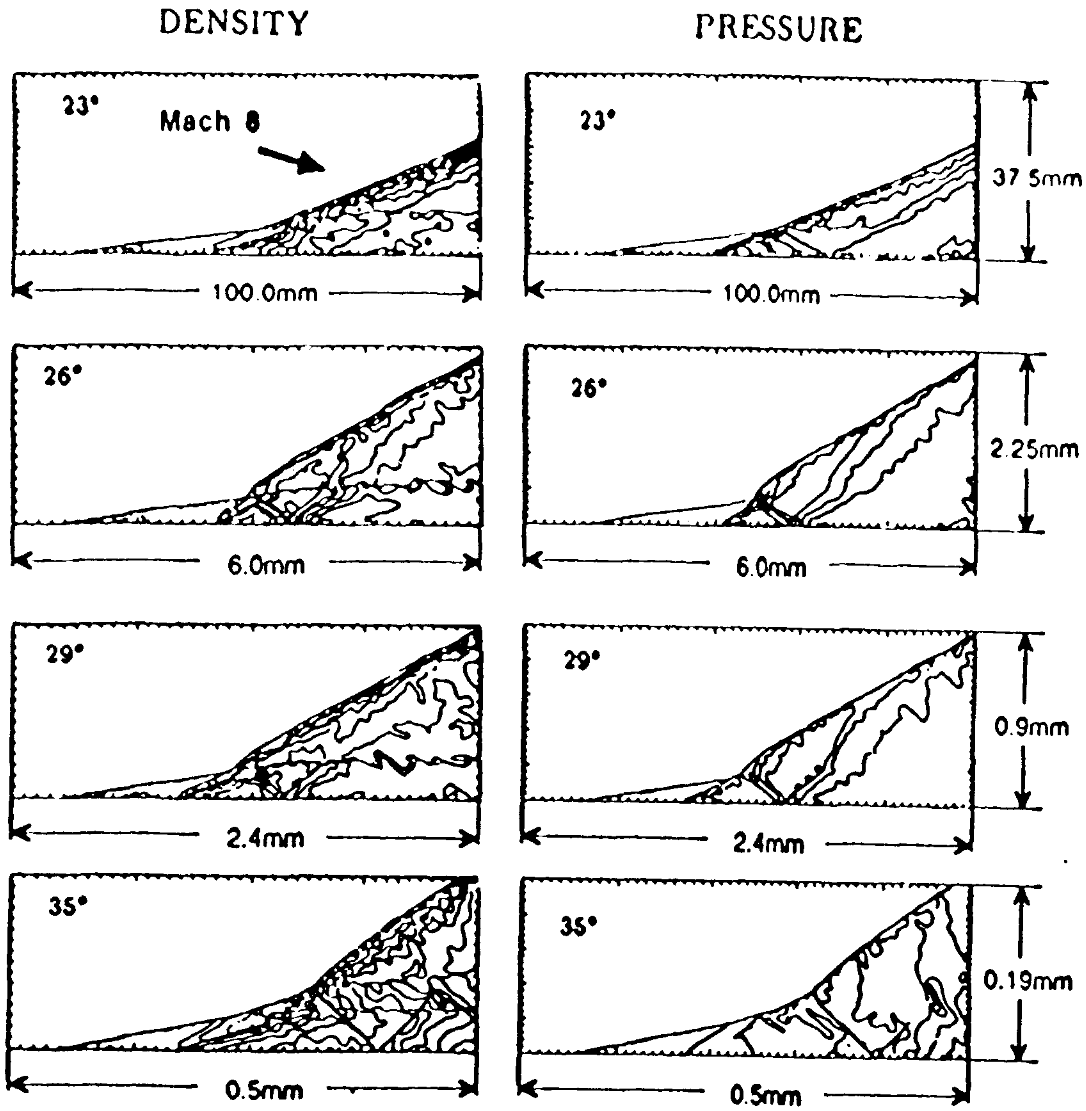


Figure 7. Detonation structures on wedges of different angles in the stoichiometric hydrogen-air mixture (H_2:O_2:N_2/2:1:3.76). The detonation structures are steady on the 23°, 26°, and 29° wedges. In the 35° case, the entire detonation structure moves continuously upstream and eventually detaches from the wedge. The bottom figure shows the evolving detonation structure at 1.25 μs from the initiation of the computation. In order to capture the detonation structure in these cases, the size of the computational domain was chosen according to these induction distances. This size varies from 100.0×37.5 mm^2 in the 23° case to 0.5×0.375 mm^2 in the 35° case, where the size in the y-direction is extended to allow the development of the upstream-moving, reactive shock. In this case, the basic structure still remains the same. However, similar to the case of H_2:O_2/2:1 discussed earlier, the whole reactive structure moves continuously upstream and detaches from the wedge. The contours shown for this case in Fig. 10 represent the evolving detonation structure at 1.25 μs from the initialization of the computation.

and the original flow field is recovered, indicating that the detonation structure is stable to such a perturbation.

The large number of simulations performed indicate that the detonation structure is stable except when the flow behind the structure is choked. For every flow configuration, there exists a maximum amount of heat that can released without choking the flow. When the energy released exceeds this value, the heated flow will no longer be able to pass through the area behind the shock, and, therefore, the shock-detonation structure is driven upstream to create a larger area to accomodate the heated flow. If a sufficiently large area of outflow cannot be generated, the entire structure will be driven out of the computational domain in a simulation or out of the test apparatus in an experiment.

Effects of Viscosity

Since the boundary layer is very thin in supersonic flows in ram accelerators, very high computational resolutions are required to conduct numerical simulations of such boundary layers. A less computationally intensive approach that can provide an estimate of the importance of boundary layers is to increase the value of the viscosity. Thus, we first performed simulations of detonation structure using different viscosity values in the same flow and mixture conditions and on the identical computational cell size, as those in the previous sections. The estimates obtained here provide a valuable guide for doing more resolved and expensive computations later.

Figure 9 shows contours of temperature and the mass fraction of water for different viscosity values. The figure shows that for the normal air viscosity, the overall detonation structure remains the same as that in the inviscid simulation. This is due to the fact that the thickness of the boundary layer is much smaller than the size of the computational cells. When the viscosity is increased by an order of magnitude, the boundary layer occupies a large portion of the first computational cell above the wall. In this case, the induction length is slightly reduced, and the whole detonation structure moves upstream accordingly. In the case of a hundred times of the normal air viscosity, the boundary layer is few cells thick, and the reduction in induction length is significant. Because the temperature is nearly constant behind the shock, we believe that the reduction in the induction distance is due to the increase in the shock strength at the leading edge rather than the viscous dissipation in the boundary layer. In the cases studied here, the temperature behind the shock is around 1200 K, and the reaction rates are very sensitive to the temperature. However, although the induction distance is reduced by the increase in viscosity, the overall detonation structure remains similar in all cases. Although the above simulations with different viscosity values show interesting effects, they can only be used as rough estimates, and more resolved computations are required to fully understand the effects of the boundary layer on the detonation structure.

In supersonic flow simulations, models such as the Baldwin-Lomax model are usually used to represent a turbulent boundary layer. Since these models are usually calibrated in different flow regimes, the validity of these kinds of models in regions where strong streamwise gradients exist (such as the nose region of the projectile) is yet to be proved. It is important to examine closely the results predicted using such models. Figure 10a shows a simulation using the Baldwin-Lomax model, and Figure 10b shows results from a numerical simulation without any explicit turbulence models. In these two cases, the overall deflagration-detonation structure remains largely intact. These results once again suggest that the boundary layer raises the temperature and pressures in the induction region by strengthening the leading shock and the dissipative heating is relatively weak. However, the simulation using the Baldwin-Lomax model shows a significantly shorter induction delay, and the overall detonation structure is established much closer to the tip of the wedge than

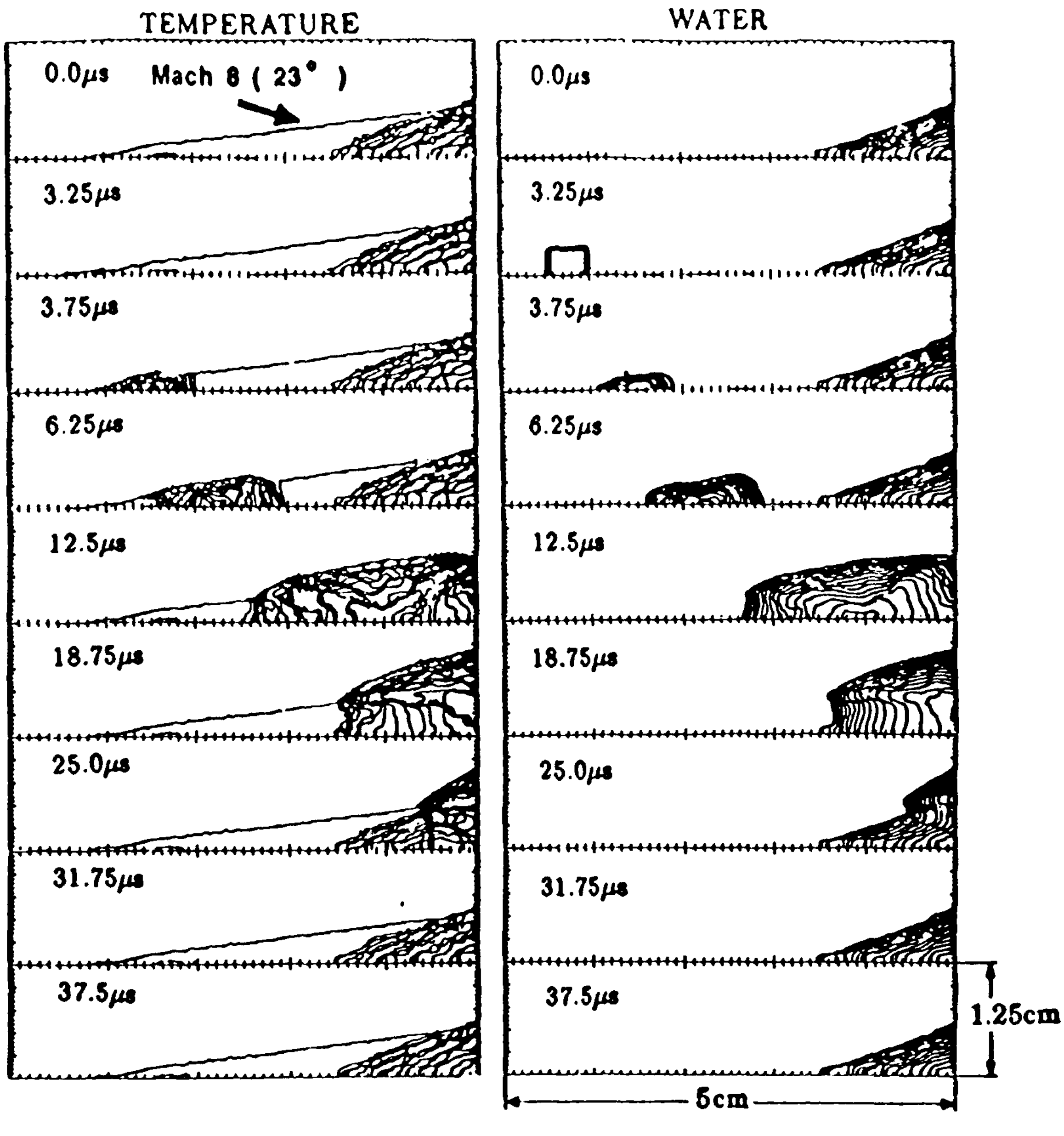


Figure 8. Development of a disturbance on the steady detonation structure.

in the inviscid simulations. The simulation without turbulence models shows less reduction in induction delay than that in the simulation using the Baldwin-Lomax model. This discrepancy is possibly due to the inability of the Baldwin-Lomax model to represent adequately the flow near the leading edge and is currently being studied in greater detail.

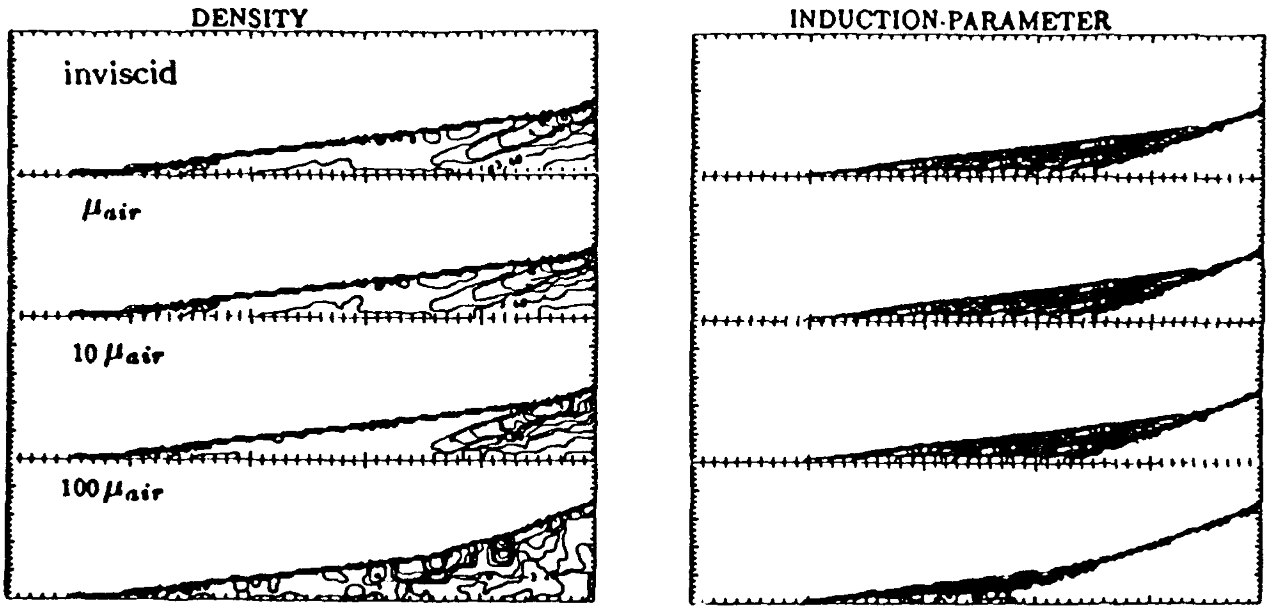


Figure 9. Simulations of detonation structure using different viscosity values.

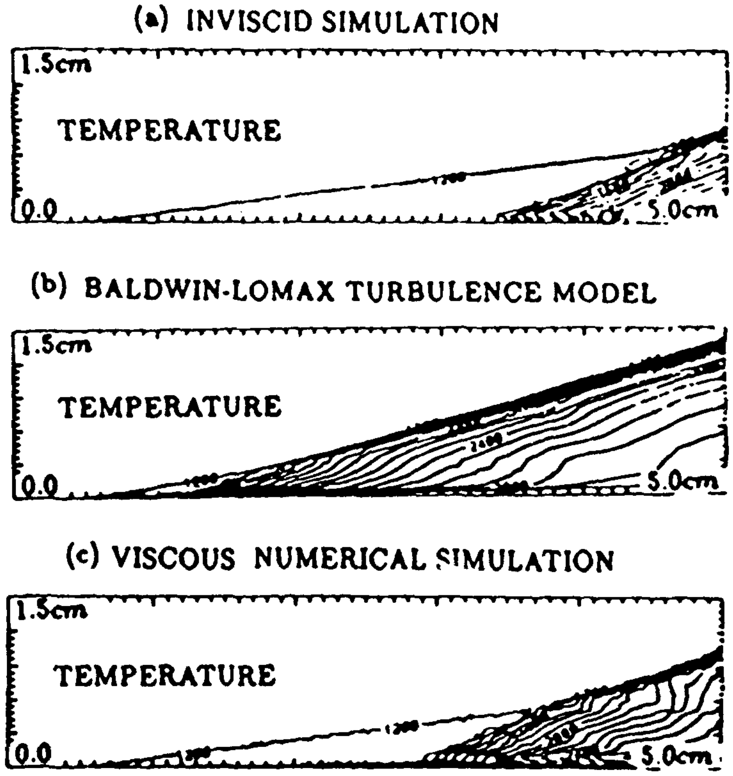


Figure 10. Oblique detonation structure predicted using different numerical models for a mixture of H_2:O_2:N_2/2:1:3.76 and in a computational domain of 5.0×1.5 cm^2.

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